Domain Structure Evolution in Thin Films

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Epitaxial $PbZr_{1-x}Ti_xO_3$ (PZT) thin films have wide applications in microwave acoustic devices, dynamic random access memories (DRAMs), ferroelectric random access memories (FeRAMs), electro-optic switches, and optical displays. However, the internal structure and thus behavior of PZT thin films can be significantly different from a bulk single crystal.

We used a phase-field model to predict the stable ferroelectric phases and domain structures at different temperatures, compositions and substrate constraints. It is found that substrate constraints may alter the ferroelectric transition temperatures by hundreds of degrees and may drastically change the phase stability, and domain structures. For example, a new ferroelectric phase-orthorhombic which does not exist in bulk PZT single crystal was automatically detected in the computer simulations.

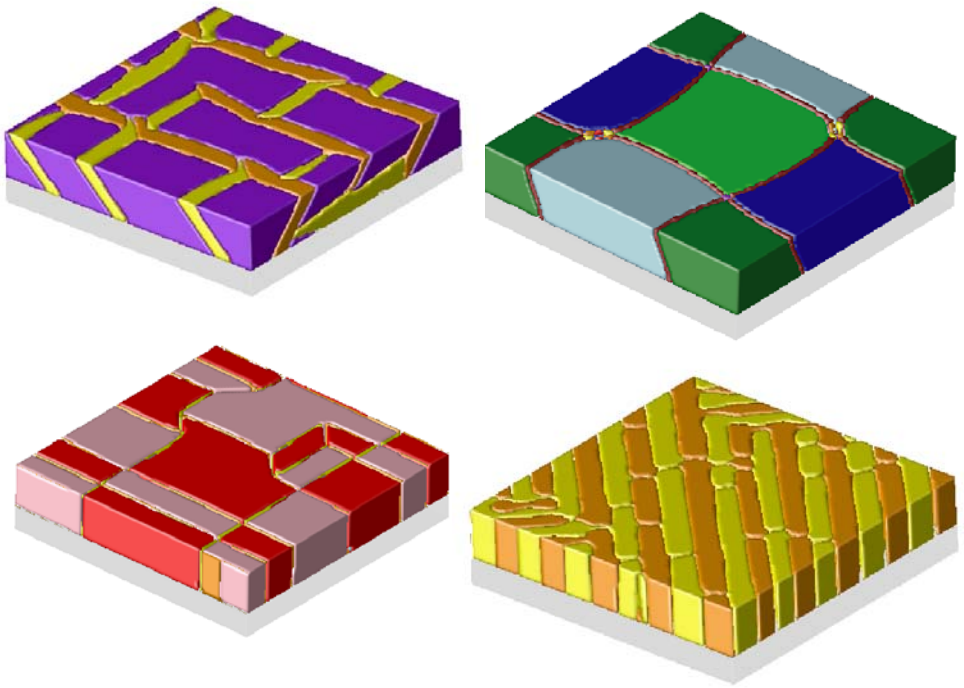

Fig. 1 shows examples of predicted different domain structures for a PZT film at different compositions or different substrate constraints. Different colors represent different domains and interfaces between them are domain walls.

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Educational Impacts

- One student and one postdoctor are currently supported by the project. Two graduate students partially supported by this project received their Ph.D. in 2002. One undergraduate student finished his B.S. thesis in 2003 and another undergraduate student worked in the project as a summer student.
- The PI taught a short course on introduction to phase-field simulation to scientists and engineers from industry, national labs and universities using the software developed in this project (Fig. 2)
- The software developed in the project have also been used in classroom demonstrations and hands-on experiences for two graduate courses and one undergraduate course.

Fig. 2. the PI was teaching a short course to scientists and engineers from industry, national labs and universities. In particular, the participants had an opportunity to perform hands-on practices on simulating microstructure evolution using the computer codes developed in this project.